

# Entanglement Simulations of Shor's Algorithm

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We demonstrate that, in the case of Shor's algorithm for factoring, highly mixed states will allow efficient quantum computation, indeed factorization can be achieved efficiently with just one initial pure qubit and a supply of initially maximally mixed qubits (S. Parker and M. B. Plenio, *Phys. Rev. Lett.*, **85**, 3049 (2000)). This leads us to ask how this affects the entanglement in the algorithm. We thus investigate the behavior of entanglement in Shor's algorithm for small numbers of qubits by classical computer simulation of the quantum computer at different stages of the algorithm. We find that entanglement is an intrinsic part of the algorithm and that the entanglement through the algorithm appears to be closely related to the amount of mixing. Furthermore, if the computer is in a highly mixed state any attempt to remove entanglement by further mixing of the algorithm results in a significant decrease in its efficiency.

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## INTRODUCTION

Quantum entanglement [1,2] is a basic resource in quantum information processing. While its role in quantum communication tasks is quite well understood the same cannot be said about quantum computation. While it is generally believed that entanglement is necessary to achieve an exponential speedup of a quantum algorithm over a classical algorithm [3] the exact mechanism by which this may happen is unclear. In fact, so far it has not been proven strictly whether entanglement is really necessary for an exponential speedup.

Generally, the argument for the power of quantum computation relies on the assumption that any algorithm that simulates the time evolution of a quantum system will be exponential in the number of quantum bits involved, if it explores the whole state space. The reason is that the dimension of the total state space of a quantum system grows exponentially with the number of subsystems. For pure states, this argument implies that the quantum system needs to evolve into an entangled state to be difficult to be simulated. If it is always in a product state, then the number of parameters required to describe it grows only polynomially with the number of subsystems. For mixed states, however, the situation changes significantly. The set of disentangled states, i.e. the separable states, has the same dimension as the set of all states, although its relative size with respect to the total state space decreases rapidly [4]. Therefore, one could imagine that there are dynamics that always leave the system in a separable state, but which are nevertheless difficult to simulate on a classical computer simply by the fact that the number of parameters that is required to describe the quantum system grows exponentially. As a consequence it may conceivably be possible to have efficient quantum computations on separable states as the

algorithm is able to efficiently simulate itself. Furthermore this points to the possibility that efficient quantum computation is possible on mixed states.

Recently Knill and Laflamme [5] investigated the power of quantum computations using one pure qubit and a supply of maximally mixed qubits and were able to construct a problem that could be solved more efficiently using these resources than any known classical algorithm. Also Schulman and Vazirani [6] were able to show that given a supply of thermal states one could produce a single pure qubit together with many maximally mixed qubits. The latter could then be discarded and the pure qubit combined with other pure qubits in a quantum algorithm. Indeed NMR quantum computation [7] does start with initially thermally mixed qubits, although the computation efficiency falls off exponentially with the number of qubits. However, we still have the possibility that these mixed qubits could be used in a useful computation like that of Knill and Laflamme. It is therefore of interest to explore this idea further and see what degree of mixing a quantum computer can tolerate before it loses its efficiency.

This paper is an exploration of this idea. We study the efficiency of Shor's algorithm when the quantum computer is in a highly mixed state. We arrive at the conclusion that Shor's algorithm can be run on extremely mixed states without significant loss of computational efficiency. Nevertheless, it turns out that despite the significant degree of mixedness Shor's algorithm runs through some weakly entangled states, leaving the question open as to whether a quantum computer really requires entanglement to be efficient.

The sections of this paper are organized as follows: in section I we give an outline of Shor's algorithm together with possible gate layouts and interpretations; in section II we examine what is known about simulating quantum algorithms; section III looks at entanglement measures

for mixed states and section IV multipartite entanglement and its quantification; sections V and VI give details of the simulations used in this work and some of the results obtained and finally section VII gives concluding remarks.

## I. OUTLINE OF SHOR'S ALGORITHM

### A. The Algorithm

Shor's algorithm for factoring an integer  $N = pq$ , where  $p$  and  $q$  are prime, relies on finding the period,  $r$ , of the function  $f_a(x) = a^x \bmod N$ , where  $a$  is some integer less than and coprime to  $N$  chosen at random. Then, with a sufficiently high probability, at least one of the unknown factors of  $N$  is given by  $\gcd(a^{r/2} \pm 1, N)$  which can be calculated efficiently using Euclid's algorithm. Classically all known algorithms are unable to solve the period finding problem in time polynomial in  $\log N$ , the length of the number being factorized.

The quantum period finding algorithm works as follows: two quantum registers are required whose state spaces are of size at least  $N^2$  and  $N$  respectively. As we will be using qubits we will require  $L = 2\lceil \log_2 N \rceil$  and  $n = \lceil \log_2 N \rceil$  of these two level systems for the two registers respectively. We initially prepare the first register in an equal superposition of all possible states by preparing each of the qubits of the register in state  $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ . The second register is prepared in state  $|1\rangle$ , where all the individual qubits are in state  $|0\rangle$  except the first which is in state  $|1\rangle$ . We now unitarily transform the two registers with the transformation  $U|x, b\rangle \rightarrow |x, ba^x \bmod N\rangle$  so that

$$U \frac{1}{\sqrt{t}} \sum_{x=0}^{t-1} |x, 1\rangle \rightarrow \frac{1}{\sqrt{t}} \sum_{x=0}^{t-1} |x, a^x \bmod N\rangle \quad (1)$$

where  $t = 2^L$ . Now, an inverse quantum Fourier transform

$$F^{-1}|y\rangle \rightarrow \frac{1}{\sqrt{t}} \sum_{z=0}^{t-1} e^{-2\pi i y z / t} |z\rangle \quad (2)$$

on the first register of Eq. 1 yields the state

$$\frac{1}{t} \sum_{x=0}^{t-1} \sum_{z=0}^{t-1} e^{-2\pi i x z / t} |z, a^x \bmod N\rangle \quad (3)$$

and the first register now contains information about the period of the function  $f_a(x)$ . We access this information by simply measuring the first register in the number, or *computational* basis obtaining the result  $|c\rangle$ , say. It was then shown in [8] that the fraction  $c/t$  is, with a sufficiently high probability, most closely approximated (using the continued fractions method [9]) by a fraction  $j/k$  (with  $k < N$ ) which in lowest terms has  $k = r$ , the period we are trying to find and will therefore sufficiently often give us a factor of  $N$ .

### B. Decomposition into basic gates

These are the essential details of Shor's algorithm as it was first formulated. We must now, of course, be sure that the algorithm runs in *time* polynomial in  $\log N$  for general  $N$  as well as using polynomial space as has been shown above. The time taken to perform the algorithm is generally assessed by counting the number of basic operations involved. To do this we must have a decomposition of the  $U$  and  $F^{-1}$  transformations into elementary gates acting on a small numbers of qubits, usually one, two or three.

One condition on these elementary gates is that each of them is reversible, that is, given the output states we could work out the input states (and obviously vice versa). The condition is imposed by the unitarity, and therefore the reversibility of the transformations  $U$  and  $F^{-1}$ . Examples of such reversible gates are CNOT's (2 qubits), TOFFOLI's (3 qubits) and an infinite variety of 1-qubit gates and 2-qubit gates where a single qubit transformation is 'controlled' by a second qubit.

Detailed polynomially efficient gate layouts for the modulo exponentiation transformations can be found in [10]. They highlight one other complication: the efficient decomposition of general unitary transformations into small basic gates seems to require auxiliary qubits. These are used during the transformation to store quantum information temporarily but are left in their initial states at the end. Some of these must be prepared in a known state ( $|0\rangle$ , say), others may be prepared in a completely unknown, or maximally mixed state which may or may not be entangled to other systems outside the computer. Either way they must be returned to their initial state after use during the computation. If they are not returned to their initial states (or some other known state that is disentangled from the rest of the computer) these qubits will be holding information about the states of the non-auxiliary qubits so that the transformation as viewed on the *non-auxiliary qubits alone* cannot be unitary or reversible and quantum information will have leaked out of the quantum computer.

A polynomially efficient gate decomposition of the (inverse) Fourier transform into 1-qubit Hadamard transformations and 2-qubit controlled phase rotations can be found in Fig. 1 and is all the gates to the right of, and including, the first Hadamard transform (H). It requires  $O((\log N)^2)$  1- and 2-qubit gates to perform the transformation and is therefore again polynomially efficient in time.

The careful (or experienced) reader will notice that for increasing  $N$  the conditioned phase rotations are of increasingly small values (controlled  $R_L = \begin{pmatrix} 1 & 0 \\ 0 & e^{-2\pi i / 2^L} \end{pmatrix}$ )

transformations are used) which would require that the accuracy of the gate implementation is exponential in  $\log N$ . This would require exponential resources (in terms of time/energy etc.) but it is clear that the Fourier transform implemented without performing the controlled phase shifts to such high accuracy does not affect the transformation too much and so does not reduce the efficiency too much. In return, however, in a practical situation involving decoherence it is an advantage not to carry out these small phase shifts as the computation will then suffer less errors due to its shorter computation time [11].

### C. The phase kickback interpretation

In Fig. 1 the controlled modulo exponentiation of the classical number  $a$  has been decomposed

into  $L$  successive controlled modulo multiplications by  $a^{2^{L-1}} \bmod N, a^{2^{L-2}} \bmod N, \dots, a^2 \bmod N, a \bmod N$  [12]. We will write these as  ${}_cU_a^{2^{L-1}}, {}_cU_a^{2^{L-2}}, \dots, {}_cU_a^{2^1}, {}_cU_a$ , where

$$\begin{aligned} {}_cU_a^{2^x} |0, b\rangle &= |0, b\rangle \\ {}_cU_a^{2^x} |1, b\rangle &= |1, a^{2^x} b \bmod N\rangle. \end{aligned} \quad (4)$$

The modulo multiplications can be written in this way, as powers of the gate  $U_a$ , because multiplication by  $a^{2^x} \bmod N$  is equivalent to multiplying by  $a \bmod N$ ,  $2^x$  times. Actually performing the modulo multiplications in this way would of course require exponentially many repetitions of the basic gate  ${}_cU_a$  and is therefore a highly inefficient method but each of the controlled modulo multiplications can be performed in time polynomial in  $\log N$  after classical precalculation of the numbers  $a^{2^x} \bmod N$  [10].

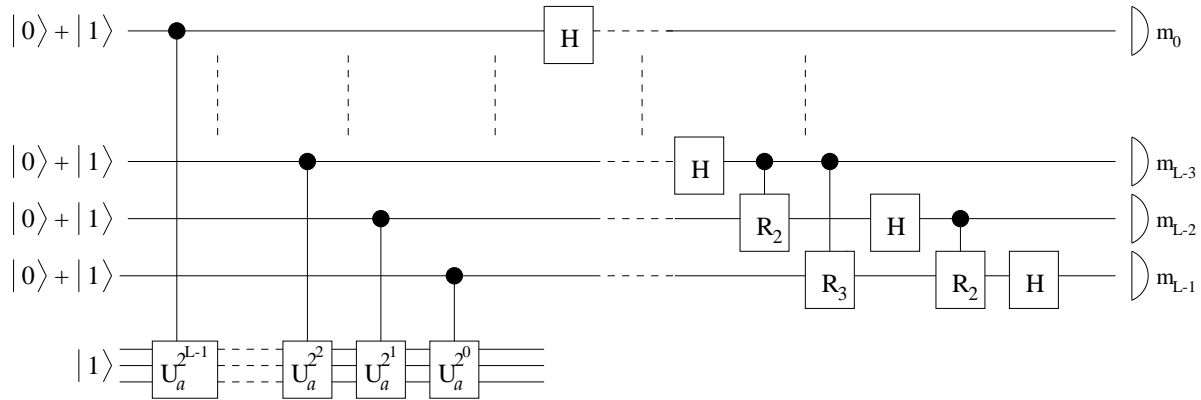


FIG. 1. An implementation of Shor's algorithm [12]. The controlled- $U_a$  operations produce controlled phase shifts related to the period of  $f_a(x) = a^x \bmod N$  and the remaining Hadamard transformations (H) and controlled rotations  $R_j = \begin{pmatrix} 1 & 0 \\ 0 & \phi_j \end{pmatrix}$  with  $\phi_j = e^{-2\pi i/2^j}$  implement the inverse Fourier transform. The result of the measurement,  $c$ , as described in section I A is given by  $c = \sum_{i=0}^{L-1} 2^i m_i$

Viewing the algorithm as such leads us to another interpretation of the period finding algorithm that is just a change of basis away from Shor's original formulation, as outlined above. The operation  $U_a$  has a set of  $r$  eigenstates  $|\psi_j\rangle$  ( $j = 0, \dots, r-1$ ) with eigenvalues  $e^{2\pi i j/r}$ . Applying a controlled- $U_a$  gate to the state

$$(|0\rangle + |1\rangle) |\psi_j\rangle \quad (5)$$

(aside from normalization) kicks the acquired phase onto the control qubit:

$$U_a (|0\rangle + |1\rangle) |\psi_j\rangle = \left( |0\rangle + e^{2\pi i j/r} |1\rangle \right) |\psi_j\rangle. \quad (6)$$

We cannot prepare the eigenstate  $|\psi_j\rangle$  as this would require knowledge of  $r$ . However, using the result  $\sum_{k=0}^{r-1} |\psi_k\rangle = |1\rangle$  [12] gives

$${}_cU_a (|0\rangle + |1\rangle) |1\rangle = \sum_{k=0}^{r-1} \left( |0\rangle + e^{2\pi i k/r} |1\rangle \right) |\psi_k\rangle. \quad (7)$$

A measurement of the control qubit, in some chosen basis, will now yield information about the fraction  $j/r$  for some  $j$  selected at random, although only one bit of information will be acquired. More information can be acquired about the phase if we perform the controlled- $U_a^{2^{L-1}}, U_a^{2^{L-2}}, \dots, U_a^{2^1}, U_a^{2^0}$  gates, using different control qubits for each, the inverse Fourier transform on the control qubits [12] and a projective measurement on each control qubit. This will sufficiently often allow us to obtain  $r$  as described above: by finding the fraction  $j/r$  closest to  $c/t$  where  $c$  is the result of the measurements on the control qubits.

Shor's algorithm, then, can be seen in terms of the pro-

duction and measurement of relative phase information which is related to  $r$ .

#### D. Using mixed states

In [13] it was shown that  $U_a$  also has other sets of eigenstates  $|\psi_{jd}^d\rangle$  ( $jd = 0, \dots, r_d - 1$ ) with eigenvalues  $e^{2\pi i jd/r_d}$  and that in fact nearly all of these (at least  $(p-1)(q-1)$  of them) have  $r_d = r$ . Consequently the lower qubits (the 2nd register) in Fig. 1 need not be prepared in the initial state  $\sum_{k=0}^{r-1} |\psi_j\rangle = |1\rangle$  but can be prepared in the completely unknown state

$$\frac{1}{N} = \frac{1}{N} \sum_{jd,d} |\psi_{jd}^d\rangle \langle \psi_{jd}^d| \quad (8)$$

(here we are equating  $|\psi_{j1}^1\rangle = |\psi_j\rangle$ ). This mixed state algorithm is run exactly as before and the period is found at least  $\frac{(p-1)(q-1)}{N}$  times as efficiently as the original pure state algorithm, this factor approaching unity as  $p, q \rightarrow \infty$ .

This also, in fact, means that any randomly selected state, whether pure or mixed, entangled or not, may be used as an input state for the lower qubits and, on average, the algorithm will run efficiently. These lower qubits may also be mixed because they are entangled to systems outside the computer [13].

In terms of the number of pure qubits that are needed in the algorithm we should once again address the matter of the decomposition of the controlled- $U_a$  transformations into basic gates (Section IB). It is well known that polynomially efficient decompositions of these transformations do exist [10] but they require auxiliary qubits which it seems need to be prepared in a pure state. With

some alterations to these decompositions, however, it has recently been shown that, of those auxiliary qubits that cannot be removed from the algorithm, only one need be prepared in a pure state [14] (this is not to be confused with the ‘one’ pure qubit of the Abstract and the next section). The rest can be prepared in maximally mixed states, although most can no longer be considered as being auxiliary to the computation.

For simplicity, however, we will not consider these auxiliary qubits or this altered form of the controlled- $U_a$  transformations for the rest of this work.

#### E. Using only one control bit

One further modification to the algorithm is to use a *semi-classical Fourier transform* [15] - notice that the gates of the Fourier transform, both one and two qubit, occur sequentially on the qubits. We could thus replace all of the first register of qubits with a single control qubit and perform the gate operations as follows (see Fig. 2): we implement the first controlled- $U_a^x$  gate and the Hadamard transformation and measure the control qubit; after resetting the state of this qubit to  $|0\rangle + |1\rangle$  we implement the next controlled- $U_a^x$  gate and replace the 2-qubit controlled phase shift with a *single* qubit phase shift *if the result of the first measurement was*  $|1\rangle$ ; we continue in this manner with a Hadamard transformation, single qubit phase shifts given the results of *all previous measurements*, and another measurement and resetting. At the end of the algorithm we have a set of measurement results that have an identical probability distribution to the algorithm using  $L$  control qubits in the first register, as in Fig. 1.

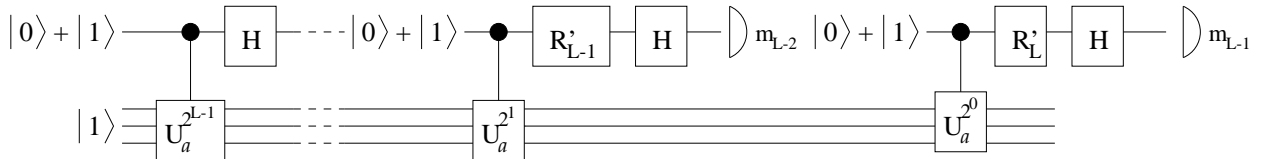


FIG. 2. An implementation of Shor's algorithm using only one control qubit which is recycled.  $R'_j$  are now combinations of the rotations  $R_j$  in Fig. 1 given the results of previous measurements:  $R'_j = \begin{pmatrix} 1 & 0 \\ 0 & \phi'_j \end{pmatrix}$  with  $\phi'_j = e^{-2\pi i \sum_{k=2}^j m_{j-k}/2^k}$ .

## II. SIMULATING ALGORITHMS

We saw in the previous section how a quantum algorithm consisting of quantum gates on quantum systems can factorize an integer  $N$  in time and number of qubits polynomial in  $\log N$ . The question then arises as to whether or not we can turn this into a classical algorithm by writing out the effect of the gates and measure-

ments on a classical system such as a computer or piece of paper. If we then find that we can do this efficiently (in time polynomial in the number of qubits) then we have an efficient classical algorithm for factoring. As no efficient algorithm is known we might be fairly certain that no such efficient simulation is possible and that all simulations of Shor's algorithm will be difficult.

Of course we already have a 'simulation' of Shor's algorithm as we have written down the equations (1) and

(3) but we cannot in general derive any of the properties of the computer, or indeed the probability distribution of the measurement results, without writing out the density matrix for the whole system (or doing something else equivalently difficult) at the relevant point.

We would like to look at the system after certain gates or sets of gates. We can easily write out the effect of a single-qubit gate  $A$  on a single qubit, whether pure or mixed, by writing down the unitary matrix for  $A$  and working out its effect on the state vector  $\mathbf{v}$  or density matrix  $\rho$ :

$$\mathbf{v}' = A\mathbf{v} \quad (9)$$

$$\rho' = A\rho A^\dagger. \quad (10)$$

However, we can only do this if the qubit is completely disentangled from other systems which we may later wish to use for information processing. This is because we clearly cannot, for example, simulate the operation of two single qubit gates on two qubits in an entangled state by tracing out the opposite qubit, implementing the gates on each and taking the combined state after the operations as the tensor product of the two states (this is not even the case if the two operations are the identity). That is, there are entries in the density matrix of the combined system which refer to the combined system rather than to the individual systems themselves.

Consider some examples in Shor's algorithm. The single-qubit gates in the Fourier transform are likely to be acting on qubits which are entangled to other qubits in the computer (possibly many of them) so to simulate the algorithm correctly we must not consider just the state of the single qubit (which will be mixed in general as it is entangled to other qubits). In contrast we noted in section ID that we may use mixed states in the lower register of Shor's algorithm and that these may be mixed because they are entangled to systems *outside* the computer. In this case we *can* address only those qubits which are within the computer, even though they may be entangled to outside systems, because we will not later be concerned with these outside systems.

Let us consider the problem in more detail, considering pure states first. The state vector of an  $M+1$ -qubit system in a general entangled state requires  $O(2^{M+1})$  complex numbers to be written down and stored [3]. If we wish to classically simulate the application of the single-qubit gate  $A$  to a qubit that is entangled to  $M$  other qubits one method of simulation would be to apply the  $2$  by  $2$  matrix representing the gate to each of the  $M$  pairs of amplitudes in state vector corresponding to different states of the remaining  $M$  qubits. This involves  $M$   $2$  by  $2$  matrix multiplications and therefore requires  $O(2^M)$  operations

So to just simulate the effect of a single-qubit transformation in general takes classical resources exponential in  $\log N$ , if entanglement exists across the  $O(\log N)$  qubits.

Of course this argument also follows for mixed states - we cannot simulate the effect of even one single-qubit gate efficiently if it is entangled to many other qubits within the computer. Using a method similar to that described above we can perform the  $2$  by  $2$  matrix multiplication on  $(2^M)^2$  blocks (pre-multiplication by  $A$  and post-multiplication by  $A^\dagger$ ) of the density matrix for the whole computer, thereby requiring  $O(2^{2M})$  operations.

But the situation here is more complicated: for pure states it is relatively easy to see if entanglement exists in a simulated algorithm (although it is by no means trivial) and whether therefore the above general method needs to be used to simulate gates acting just on parts of the computer. For mixed states, however, it is harder to determine which qubits are separable. For two qubits to be separable there must *exist* a decomposition into pure states where the pure states are all separable:

$$\begin{aligned} \rho_{12} \text{ separable} &\Leftrightarrow \exists |\psi_i\rangle_{12}, p_i (> 0) \text{ such that} \\ \rho_{12} &= \sum_i p_i (|\psi_i\rangle\langle\psi_i|)_{12} \text{ where} \\ \forall i |\psi_i\rangle_{12} &= |\psi_i^1\rangle_1 \otimes |\psi_i^2\rangle_2 \end{aligned} \quad (11)$$

For almost all states there will be a decomposition into non-separable states. Finding a separable decomposition however, and indeed finding if it exists, is a difficult task.

A mixed state algorithm, then, may be seen as a mixture of pure state algorithms and even if at each stage these pure state algorithms are entangled there may exist other sets of pure state algorithms which are not entangled which mix to give the same mixed state algorithm. And these disentangled sets of pure algorithms will be different after each gate so we cannot easily preclude one existing [16].

### III. ENTANGLEMENT MEASURES AND MIXED STATES

#### A. Entanglement measures for pure states

Let us first deal with how we would measure entanglement between two quantum systems whose combined state is pure. Many entanglement measures in some way view entanglement as a resource. The process of teleportation [17,18] is an important example of a phenomenon that requires entanglement to be observed at all, as it is required in many other applications of quantum information processing including entanglement swapping, dense coding, precision measurements and hiding classical information [17,19] and in the violation of Bell's inequalities [20].

To do perfect teleportation of an unknown single qubit state requires one of the four Bell states (or 'EPR pairs') (Eq. 12 and 13) to be shared between the two separated parties 1 and 2:

$$|\phi_{12}^{\pm}\rangle = \frac{1}{\sqrt{2}}(|0\rangle_1|0\rangle_2 \pm |1\rangle_1|1\rangle_2) \quad (12)$$

$$|\psi_{12}^{\pm}\rangle = \frac{1}{\sqrt{2}}(|0\rangle_1|1\rangle_2 \pm |1\rangle_1|0\rangle_2). \quad (13)$$

Any other state of two qubits (which cannot be transformed into one of the above by unitary transformations performed by the two parties separately) cannot be used to perform teleportation perfectly.

To quantify the entanglement of a general state  $|\psi\rangle_{12}$  we could look at how well they perform the teleportation process (with some sort of 'fidelity' measure between the input state and the output state or the maximum probability for perfect teleportation). In fact, we would rather ask how many Bell states can be obtained from the given state  $|\psi\rangle_{12}$  using only Local quantum Operations (such as transformations, addition and removal of local separable systems and measurements) and Classical Communication (LOCC for short) [21]. The Bell states, therefore, have entanglement of value '1' because you can only obtain one Bell state from each Bell state supplied (you cannot on average increase the number of Bell states with LOCC).

For other states of two qubits, say

$$|\psi\rangle_{12} = a|00\rangle_{12} + b|11\rangle_{12}, \quad a, b \in \mathcal{R}^+, \quad a > b, \quad (14)$$

(with  $a^2 + b^2 = 1$ ) let us consider first what we can do with just one copy of the state. The most efficient method of obtaining a Bell state from this state is to use the Procrustean method [21–23]. This only creates a Bell state with probability  $2|b|^2$ , the rest of the time creating a completely separable state.

We can do better than this efficiency if we are supplied with more copies,  $n$  say, of the state  $|\psi\rangle_{12}$  held by the separated parties. Now we can increase the number of Bell states obtained between the parties *per copy* of  $|\psi\rangle_{12}$  held by allowing each of the separated parties to perform *joint* operations on those parts of the entangled states each holds. So say  $k$  is the number of Bell pairs obtained, then on average, and with a suitable method,  $k/n \geq 2b^2$ . The exact results for any finite number of copies are known [23] and asymptotically, in the limit of large  $n$  (provided we allow an arbitrarily small probability of error), the average number of Bell pairs obtained per copy for pure states is given by

$$\frac{k}{n} = E(\rho_{12}) = S(\rho_1) = S(\rho_2) \quad (15)$$

where  $\rho_{12} = (|\psi\rangle\langle\psi|)_{12}$ ,  $S(\sigma)$  is the von Neumann entropy of the density matrix  $\sigma$ , and  $\rho_1$  and  $\rho_2$  are the partial density matrices of the first and second of the entangled particles. For the state of Eq. (14) this gives  $E((|\psi\rangle\langle\psi|)_{12}) = -a^2 \log a^2 - b^2 \log b^2 > 2b^2$ . These, and future results also hold for two party systems composed of individual systems of more than two levels.

In the asymptotic limit (only) the process is also true in reverse: given  $k$  Bell pairs and taking  $k \rightarrow \infty$  we can create from them, using LOCC,  $k/E(\psi_{12}) = n$  copies of the state  $|\psi\rangle_{12}$ . We say, then, that for pure states the asymptotic *entanglement of formation*,  $E_F$  (the number of Bell states we need to pay per copy of state  $|\psi\rangle_{12}$  we get in return) [24,25], is the same as the asymptotic *distillable entanglement*  $E_D$  (the number of Bell pairs we can distill out of the state  $|\psi\rangle_{12}$  per copy of  $|\psi\rangle_{12}$  paid).

## B. Mixed states

For mixed states the situation is far less clear.  $E_F$  and  $E_D$  can be defined in the same way but for general mixed states they are not equal - you cannot in general get as many Bell pairs out of a state as you would put in (you certainly cannot obtain more or you would be able to locally create entanglement *ad infinitum*). This is due to the fact that a mixed state is to some extent unknown and the randomness inserted on the formation of the state from Bell states cannot be eliminated unless extra information about the state is obtained.

Another problem with  $E_F$  and  $E_D$  defined in this way is that at present there are no analytical methods for calculating either for general mixed states. The only example where an analytical expression does exist for more than some specific subclasses of states is the entanglement of formation of a single two-qubit system [25].

These entanglement measures are not the only possibilities we could produce. Others exist such as the relative entropy [26]. So what are the conditions for a mathematical object to be called an entanglement measure? One set of conditions that are generally accepted as being sensible for an entanglement measure of a state  $\rho_{12}$  are as follows [27]:

- (i)  $E(\rho_{12}) = 0$  if  $\rho_{12}$  is separable.
- (ii) Local unitary transformations on  $\rho_{12}$  leave  $E(\rho_{12})$  invariant, i.e.  $E(\rho_{12}) = E(U_1 \otimes U_2 \rho_{12} U_1^\dagger \otimes U_2^\dagger)$ .
- (iii)  $E(\rho_{12})$  cannot, on average, increase under local operations and classical communication.

We may also wish to add one more condition to this list. This says that

- (iv) the entanglement measure should be equal to the pure state entanglement measure (Eq. (15)) for all pure states.

Of course not all entanglement measures need obey this condition, indeed the one we will be using below does not. There are many candidates for entanglement measures and all these measures will not agree with each other for mixed states. More importantly, the measures will put a different *order* on the states [28,29], that is, according to one measure of entanglement  $E_1$  the state  $\rho_{12}$  may be more entangled than  $\sigma_{12}$  but according to another measure of entanglement  $E_2$  the state  $\sigma_{12}$  could be

more entangled than  $\rho_{12}$ :

$$\begin{aligned} E_1(\rho_{12}) &> E_1(\sigma_{12}) \\ E_2(\sigma_{12}) &> E_2(\rho_{12}). \end{aligned}$$

Indeed, it was shown in [28] that any two entanglement measures that agree for pure states but not for mixed states *must* put a different order on the states.

We must accept, then, that entanglement measures may put different orders on states. The only alternative is to declare one entanglement measure as the 'correct' one, which immediately prevents us from examining how we might prepare entanglement and how we might use it.

### C. A measure of entanglement for mixed states

For the present work we need a measure that is easy to calculate and has an analytical form for general mixed states. We will call this measure the *logarithmic negativity*  $E_{neg}$  [30–32]. It is defined as follows: first denote the matrix elements of the density matrix  $\rho_{12}$  in some tensor product basis by

$$\rho_{12}^{ij,kl} = {}_1\langle i| {}_2\langle j| \rho_{12} |k\rangle_1 |l\rangle_2. \quad (16)$$

The *partial transpose* [33] with respect to system 2 is then defined in this notation as

$$\left(\rho_{12}^{T_2}\right)^{ij,kl} = \rho_{12}^{il,kj} \quad (17)$$

(the labels  $l$  and  $j$  have swapped places). It has been shown [33] that the positivity of this new matrix (that is, the positivity of all its eigenvalues) is a necessary condition for the state to be separable. Therefore,  $E_{neg}$  is now defined as the log of the sum of the absolute values of the eigenvalues of the new matrix  $\rho_{12}^{T_2}$  or  $\rho_{12}^{T_1}$  (the eigenvalues and therefore this measure are also independent of the particular tensor product basis in which the state is considered). This can be written in more compact form as

$$E_{neg} = \log \text{Tr}|\rho_{12}^{T_2}| = \log \text{Tr}|\rho_{12}^{T_1}|. \quad (18)$$

As mentioned above this measure does not agree with the pure state entanglement measure of Eq. (15). However, one particularly useful property of  $E_{neg}$  is that it is an upper bound for  $E_D$ :

$$E_{neg} \geq E_D. \quad (19)$$

What is more important is that if  $E_{neg} = 0$  we can be sure that the two party system does not have distillable entanglement, although it is not known whether the reverse statement is true or not: we cannot say that distillable entanglement does exist if  $E_{neg} \neq 0$ . Also the fact that  $E_{neg} = 0$  does not mean that the state is separable (there exist states with  $E_{neg} = 0$  that are inseparable, which are known as *bound entangled states* [34] as the entanglement cannot be distilled into Bell states but is somehow bound from us).

## IV. MULTIPARTITE ENTANGLEMENT

Entanglement does not only exist between two-party (bipartite) systems, it can also exist between three or more parties. One example is the three-party GHZ state [35]:

$$|\psi_{GHZ}\rangle_{123} = \frac{1}{\sqrt{2}}(|0\rangle_1|0\rangle_2|0\rangle_3 + |1\rangle_1|1\rangle_2|1\rangle_3). \quad (20)$$

One particular property of this state is that it has no bipartite entanglement in the sense that if we trace out the third party, say, the remaining bipartite state is given by

$$\begin{aligned} &\text{Tr}_3(|\psi_{GHZ}\rangle\langle\psi_{GHZ}|)_{123} \\ &= \frac{1}{2}(|0\rangle_1\langle 0| \otimes |0\rangle_2\langle 0| + |1\rangle_1\langle 1| \otimes |1\rangle_2\langle 1|). \end{aligned} \quad (21)$$

The entanglement in this state is of different nature to the one contained in an EPR state because it is impossible to inter-convert GHZ states and EPR pairs reversibly [36]. While one can create a GHZ state from two EPR pairs, one can only ever obtain one EPR pair from one GHZ state. What is not known for three party systems is whether GHZ states and EPR pairs are the only different kinds of entanglement. What is known is that there are in fact more types of multipartite entanglement for systems of *more* than three parties [37–39]. Three-party entanglement, then, may contain two-party entanglement and under certain conditions we can locally reversibly (under LOCC) transform between the two [40].

How then do we measure the entanglement of a multipartite system? Because of the different types of entanglement involved having one general measure for all these types is difficult (the relative entropy suitably redefined for multipartite systems is perhaps one exception [41] although there are still many problems).

Our approach will be to use a bipartite entanglement measure to verify the existence of entanglement between all the different qubits in the computer. Let us suppose that we have an entanglement measure for bipartite systems, or a way of verifying whether a state is separable or not between the two parts of the bipartite system. We now use this measure on all possible bipartite partitionings of an  $n$ -party system. For example, for a system of 4 qubits labeled as 1, 2, 3, and 4 the possible bipartite partitionings are

$$\begin{aligned} &1/234, 2/134, 3/124, 4/123, \\ &12/34, 13/24, 14/23 \end{aligned}$$

where  $1/234$  means system 1 is considered as being partitioned from systems 2, 3 and 4. For general  $n$  there are  $2^{n-1} - 1$  such partitionings.

Clearly, if there is entanglement between the two sides for at least one partitioning, then the state is entangled. The question remains as to whether the converse is true, that is, if all bipartite partitionings are separable is the state completely separable i.e. the multipartite state can be written as a mixture of product states? For pure states it is clear that this is also true (in fact, you need only look at some particular subset of the possible partitionings). But for mixed states it is *not* true - there are states that are separable across all bipartite partitionings (and therefore have positive partial transpose (PPT)) but that are not completely separable [42]. However this entanglement cannot be distillable entanglement - if we could distill it into pure multipartite entanglement by local operations it could in turn be changed into bipartite entanglement between qubits.

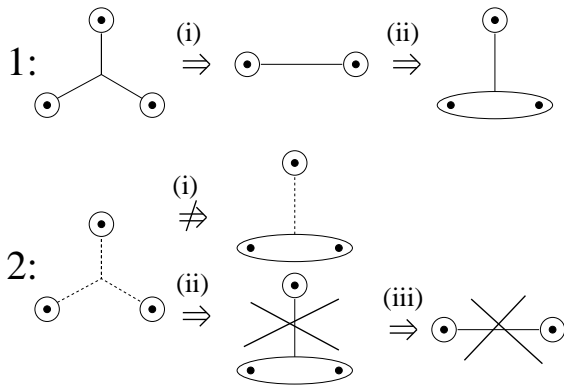


FIG. 3. Diagram outlining the possible entanglements for a multi-particle system, here for three parties. (1.) A three-party state which has distillable entanglement (solid line) (1.i.) can always be transformed into two-party distillable entanglement (at least some of the time). (1.ii.) This in turn means that distillable entanglement must exist across a bipartite boundary (one in some way separating the two parties who can obtain the two-party entanglement above) simply because allowing the third party to combine his operations non-locally with one of the other two is a more powerful operation. However, (2.) three-party non-distillable entanglement (dashed line) (2.i.) may or may not contain non-distillable entanglement between a two-party partitioning, although (2.ii.) it certainly does not contain distillable entanglement of this form and therefore (2.iii.) no distillable entanglement of any sort exist between two parties.

Our method in the simulations, then, will be to use the *logarithmic negativity* measure across all bipartite partitionings of the qubits in the algorithm. This will tell us if any distillable bipartite entanglement exists in the algorithm but will also show us if distillable multipartite entanglement of any form exists. This follows from the fact that this measure in effect verifies whether the state is PPT and is therefore not distillable across any bipar-

tite partitioning. If this is the case then no multipartite distillable entanglement can exist (we cannot distill the entanglement into pure state entanglement) otherwise we would again be able to distill this into (pure) bipartite entanglement of some form.

So, we can indeed verify in this way whether any distillable entanglement of any form exists although we cannot preclude that there exist non-distillable entangled states.

## V. THE SIMULATIONS

### A. The Basic simulations

Let us first introduce the basic method of our simulations. The states and gates are all stored in matrix form, the former as density matrices (because we will in general be using mixed states) and the gates as specific unitary transformations.  $n$  qubits therefore require  $2^n \times 2^n$  density matrices and unitary transformations. After inputting the initial state of the computer we simulate the effect of each gate by pre- and post-multiplying the density matrix by the unitary transformation and its Hermitian conjugate representing the gate to obtain the new state of the computer.

#### 1. Simulation of quantum gates

We will not simulate the effect of all single-, two- or three-qubit gates but will only simulate the algorithm as it appears in Figure 2 where we have convenient points at which to examine the computer i.e. we will only simulate the controlled modulo multiplication gates as a single gate and the gates of the Fourier transform. We will also be using this version of the algorithm as it reduces the number of qubits needed (by about 2/3) which will result in a great decrease in time and space resources the algorithm requires to be simulated.

It was noted in section II that, in general, because of the potential entanglement across all the qubits in the algorithm, the simulation of even a single qubit gate requires an exponential number of operations. For example, if the single qubit Hadamard transform

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad (22)$$

is acting on the first qubit in a computer consisting of 2 qubits then the unitary transformation required is

$$H \otimes \mathbf{1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{pmatrix}, \quad (23)$$

and if it is acting on the second qubit



$$1 \otimes H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix}. \quad (24)$$

To simulate the effect of these gates on the 2 qubit state by straight matrix multiplication however is not optimal. From the form of the above transformations it is clear that it is better to act with the Hadamard transform on blocks. In the case of  $H$  acting on the first qubit the density matrix written in block form evolves as

$$\rho = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \rightarrow \begin{pmatrix} HAH^\dagger & HBH^\dagger \\ HCH^\dagger & HDH^\dagger \end{pmatrix}. \quad (25)$$

Here of course  $C = B^\dagger$  (saving us some calculation time) as it is a density matrix and also for the Hadamard transformation  $H = H^\dagger$ . The same is true for  $H$  acting on the second qubit except the elements in the 2 by 2 blocks upon which  $H$  acts (within the 4 by 4 density matrix) are separated as is shown diagrammatically here:

$$\begin{pmatrix} a & b & a & b \\ c & d & c & d \\ a & b & a & b \\ c & d & c & d \end{pmatrix} \quad (26)$$

(lower case letters correspond to elements of blocks).

For a general  $2^n$  by  $2^n$  density matrix the simulation of a single qubit gates thus requires  $O(2^{2n})$  operations. For gates acting on  $m \leq n$  qubits this number rises to  $O(2^{2n+m})$  operations.

## 2. Simulation of tracing and measurements

First of all we may need to trace out one (or more) of the qubits (labeled by  $x$ ) of the computer to leave the density matrix

$$\rho_{12 \dots (x-1)(x+1) \dots n} = \text{Tr}_x(\rho_{12 \dots n}). \quad (27)$$

In matrix form this tracing step effectively involves adding two  $2^{n-1}$  by  $2^{n-1}$  sub-matrices together and zeroing the rest of the  $2^n$  by  $2^n$  matrix. Thus the tracing step requires  $O((2^n)^2)$  operations (although these operations are additions rather than multiplications and are therefore considerably quicker).

We can simulate single-qubit projective measurements in a similar way to that of simulating gates. We will assume, without loss of generality, that all measurements are done in the computational basis, as to perform a measurement in a different basis (even an entangled basis) we can unitarily transform the system (with entangling gates if necessary) and measure in the computational basis.

First of all we must calculate the probabilities of a measurement on the qubit yielding the result  $|0\rangle$  ( $p_0$ ) or

$|1\rangle$  ( $p_1 = 1 - p_0$ ). This is done by summing those elements on the diagonal of the density matrix for the whole computer which correspond to the measurement result.

For a Monte Carlo simulation of measurement results we may now generate a random number,  $p$ , from a uniform linear distribution between 0 and 1, and if  $p < p_0$  take the simulated measurement result to be  $|0\rangle$ , otherwise it is  $|1\rangle$ .

The measurement changes the state of the computer. To simulate this we must use two projection operators

$$P_0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \text{ and } P_1 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad (28)$$

and act on the state with either  $P_0$  (if the measurement result was  $|0\rangle$ ) or  $P_1$  (if the result was  $|1\rangle$ ) just as we would act with a single qubit gate. This will, of course, result in just setting 3/4 of the element of the density matrix to zero. This gives us the (subnormalised) state of the measurement collapsed computer, including the (partial or total) collapse of any qubits that are entangled to the measured qubit.

We must then be sure to renormalize the state of the whole computer. This can be done easily by dividing each entry of the density matrix for the collapsed computer by the trace of the density matrix (or equivalently the measurement probabilities,  $p_0$  or  $p_1$ ).

The simulation of the measurement therefore takes  $O(2^{2n})$  operations but notice that the quantum computer does this in linear time, as it only needs to find qubit  $x$  and measure it.

For the full Monte-Carlo type simulation we must of course repeat the simulation of the algorithm a number of times and average any properties of the system we obtain during each simulation.

## 3. Other processes

We can also re-prepare the measured qubit in the required state using this method by another application of single qubit gates. If we wish to prepare the state  $|0\rangle + |1\rangle$  then if the measurement result was  $|0\rangle$  we apply  $H$  and if it was  $|1\rangle$  we apply a state flip  $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$  followed by  $H$ .

We can now simulate any algorithm we wish with any set of gates and any type of measurement (a Positive Operator Valued Measure (POVM) can be simulated by adding auxiliary systems, performing unitary transformations on these systems together with the computer and measuring the auxiliary systems).

#### 4. Entanglement calculations

We are mainly interested in the degree of entanglement at each stage. As mentioned in section III B the degree of entanglement does not change under local unitary operations so we need only examine the entanglement after operations on more than one qubit. From Fig. 2 this will be after the controlled- $U_a$  operations (where entanglement may increase or decrease) as well after the measurements (where the entanglement may also increase or decrease but *on average* it should never increase - local projective operations can never increase the amount of entanglement on average).

As in section IV we will use the logarithmic negativity measure of section III C, calculated and averaged across all possible bipartite partitionings of the system. If we are using a Monte Carlo simulation these must of course be averaged across repeated simulations of the algorithm as different entanglements will be observed with different measurement results.

#### 5. Efficiency Accountancy

Let us now check the time efficiency (or lack of it) of Shor's algorithm simulated by the above method:

(i) to form those gates acting on all qubits requires  $O(2^{2n})$  steps and there are  $O(n)$  of these giving  $O(n2^{2n})$  steps altogether

(ii) for these gates the matrix multiplications for the simulation of the gate require  $O(2^{3n})$  operations. There are  $O(n)$  of these gates giving  $O(n2^{3n})$  operations in all.

(iii) each application of a single qubit gate (including measurement projections) takes  $O(2^{2n})$  steps and there are  $O(n)$  of these, which is  $O(n2^{2n})$  operations altogether.

(iv) at  $O(n)$  of the steps we wish to examine the entanglement  $O(2^n)$  times. This requires  $O(2^{2n})$  steps each for the partial transposition,  $O(2^{3n})$  for the numerical eigenvalue routine [43] and  $O(n)$  steps for the remaining calculation of our entanglement measure. From the most inefficient process (numerical eigenvalue calculation) this gives  $O(n2^{4n})$  operations for the whole. This then is the most important stage of the simulation in terms of the efficiency of the algorithm.

#### B. Tree simulations

In the above accounting we have not included any contribution from the fact that we have to repeat the whole simulation many times for the Monte Carlo method (section V A 2). Let us examine this more carefully. If we wish to estimate the probability distribution  $\{P, 1 - P\}$  with two possibilities to a certain accuracy,  $\epsilon$ , we must

repeat the Monte Carlo simulation approximately some number  $T(\epsilon)$  times. At the  $j^{th}$  measurement of the algorithm there would be  $2^{j-1}$  states the computer could be in at the point (from the previous possible measurement results). For each of these we would need to estimate the probability distribution giving  $2^{j-1} \times T(\epsilon)$  simulations we need to perform, this number getting exponentially worse at each step. So, given a fixed number of simulations the accuracy of the probability estimate and therefore the estimate of any properties of the system can get exponentially worse at each measurement step.

This leads us to an alternative simulation method, a 'tree' type simulation where every possibility of each measurement is considered. We have  $L$  measurements during the algorithm and at each one the algorithm is given two possible 'paths' to use for each of the paths already available. So the computer can take two different paths (be in two different states) at the first measurement, four different paths at the second and  $2^L$  ( $L = 2n$ ) different paths after the last measurement. This gives us  $2^{2n+1} - 1$  possible states of the computer through the algorithm. And we want to sample the entanglement in the computer at two stages between each measurement, after the measurement and after the controlled modulo multiplication gates.

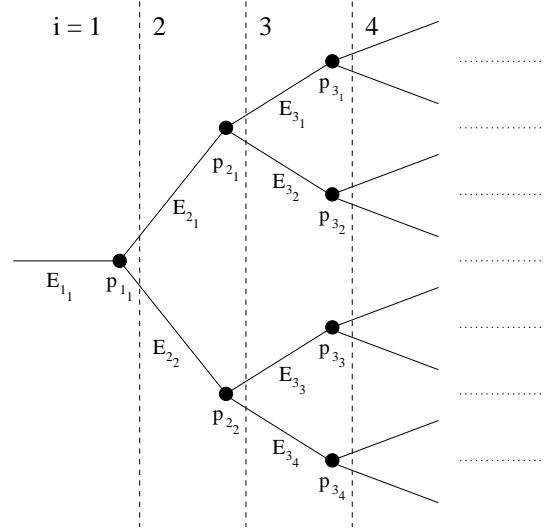


FIG. 4. The 'tree' method of simulating an algorithm.  $p_{ij}$  are the probabilities for obtaining a measurement result  $|0\rangle$  for the  $j^{th}$  branch before the  $i^{th}$  measurement ( $j = 1 \dots 2^{i-1}$ ). Likewise,  $E_{ij}$  are the values of some property,  $E$ , of the system for the  $j^{th}$  branch before the  $i^{th}$  measurement. The average of the property before the  $i^{th}$  measurement is therefore  $E_i^{av} = \sum_{j=1}^{2^{i-1}} \left( \prod_{k=1}^{i-1} p_{k_{\lceil j/2^{i-k} \rceil}} E_{ij} \right)$ .

We can calculate the probability of each of the measurement results at each stage of the algorithm and find the probability for each possible path leading to that stage. Having calculated these we can calculate exact averages for any properties of the system at any stage

if we know the properties we wish to examine at each branch of the tree.

This gives us, of course, another exponential overhead in our simulation but, as we saw, this was the same for the Monte Carlo simulation.

### C. Noise simulation

The high susceptibility of quantum computers to noise from the environment [44] in which the computer is run has been known for some time. This noise comes from entanglement of the computer with the environment suffered during the execution of the algorithm. Further sources of error are inaccuracies in the measurements and implementation of the gates. Fortunately it has been shown that *error-correcting codes* exist [45]. These encode the state of a qubit into the joint (entangled) state of many qubits such that random errors occurring independently on the qubits below a certain (reasonable) threshold can be corrected back to the correct state using measurements and unitary transformations based on the measurement results. It has also been shown that these codes can be used in *fault tolerant* quantum error correcting schemes [46], that is, the measurements and transformations that implement the error correcting code itself need not be implemented perfectly.

The fact that Shor's algorithm can be implemented with 'noisy' mixed states leads us to asking if this in any way increases the algorithm's robustness to noise, or whether the coherence within the pure state decomposition of the mixed states needs to be preserved.

It will be interesting, then, to simulate the effects of random noise injected into the computer and its effect on the efficiency with which the number  $N = pq$  is factorized.

There are many ways of simulating noise and many types of noise we could use in the simulation. We have selected two types, noise by measurement and noise by random Pauli operations. It should be noted, however, that different types of noise, whether in quantum or classical scenarios, tend to have similar qualitative effects and so we need not worry too much about the precise nature of each.

#### 1. Noise by measurement

Here, we address each qubit in turn and with a given probability apply a measurement on that qubit in the computational basis (although it need not be in this basis for general noise). The probability for the two outcomes is governed by the state of the particle, as described in section V A 2.

This collapses the state of the computer in some way. We will, with the given probability, apply the noise step

to every qubit after each gate during the algorithm. Of course, the controlled modulo multiplication gate consists of many gates acting on small numbers of qubits so would have more time to be effected by noise.

We should also carefully note that when running the algorithm we would not know the result of the measurement taken by the measurement noise and the algorithm would at that stage become more mixed (the computer becomes a weighted mixture of the two states post measurement) as we do not know which measurement result was found. In fact we would not even know if a noise step had been applied.

#### 2. Noise by Pauli operations

Here, again addressing each qubit in turn, with a certain probability we will apply one of the three Pauli operators ( $\sigma_x, \sigma_y, \sigma_z$ ), or the identity operator ( $I$ ):

$$\begin{aligned}\sigma_x &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \sigma_z &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\end{aligned}\quad (29)$$

to the qubit, these four operations occurring with equal probability.

Again we should be careful to point out that a noise step would leave the computer in a equal mixture of the four states that result after the application of the four Pauli operations. Thus the qubit will have its state completely randomized (although it could still be entangled to other qubits).

### D. Mixing of the control qubit

As we want to examine the entanglement in the computer it will be interesting to investigate ways of reducing the entanglement and seeing how this affects the computer. We have already introduced mixed states into part of the quantum computer and seen that it does not affect the efficiency very much. But we could also mix the state of the control qubit. This must affect the efficiency of the algorithm (a totally random algorithm cannot be any use to us) and it will be useful to compare this to the change in entanglement.

We will do this by preparing (and re-preparing) the control qubit in the state

$$(1 - \epsilon) |\psi\rangle \langle\psi| + \epsilon |\psi^\perp\rangle \langle\psi^\perp| \quad (30)$$

where  $|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$  and  $|\psi^\perp\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$ . Using the methods of our quantum computer simulator this tensor product operation is most conveniently done as follows: we assume that the control qubit is in state

$|0\rangle$  (if it is in the state  $|1\rangle$  after measurement it can be flipped easily); if we denote the state of the whole computer (including the control qubit) by  $\rho_{12\dots n}$  we calculate the temporary density matrix

$$\rho_{12\dots n}^t = (F \otimes \mathbf{1}^{n-1}) \rho_{12\dots n} (F \otimes \mathbf{1}^{n-1}); \quad (31)$$

where  $F$  denotes the single qubit flip operator (section V A 3); we can then mix this with the original density matrix for the computer in the required proportions:

$$\rho_{12\dots n}^{mix} = (1 - \epsilon)\rho_{12\dots n} + \epsilon\rho_{12\dots n}^t \quad (32)$$

and a final Hadamard transformation on the control qubit gives us the required state of the computer.

Changing the parameter  $\epsilon$  between 0 and 1/2 allows us to decrease or increase the mixedness of the computer.

## VI. RESULTS

### A. Entanglement in Shor's algorithm

Firstly we will look at the entanglement in the pure and mixed state single control qubit algorithms (calculated using the 'tree' simulation method (section V B)). We will look at the average bipartite entanglement as measured by the logarithmic negativity entanglement measure (section III C) averaged across all possible bipartite boundaries at each stage of the algorithm (section IV). We will also average across all possible algorithms factorizing numbers of 4 binary digits and 5 binary digits. These results are shown in Figs. 5 and 6.

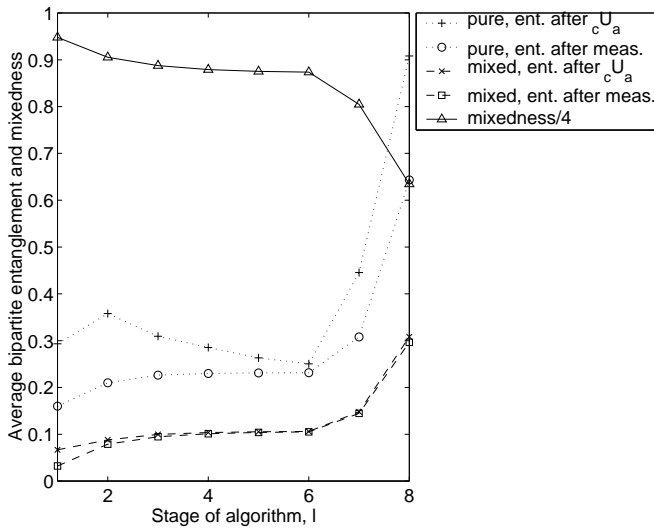


FIG. 5. The average bipartite entanglement measured by the *logarithmic negativity* measure vs. the stage of the algorithm for both pure and mixed state algorithms. The average entanglement is given after  $s^{th}$  controlled modulo multiplication gate and after the  $s^{th}$  measurement. This average is an average entanglement over all bipartite partitionings of the  $n$ -qubit system as well as over all algorithms for factorizing numbers which are products of two primes and have four binary digits (i.e. 9, 10, 14 and 15) and over all possible numbers  $a$  coprime to each of these numbers. Also shown is the mixedness (divided by 4) after the  $s^{th}$  measurement. Notice how this closely mirrors the entanglement in the mixed state algorithm.

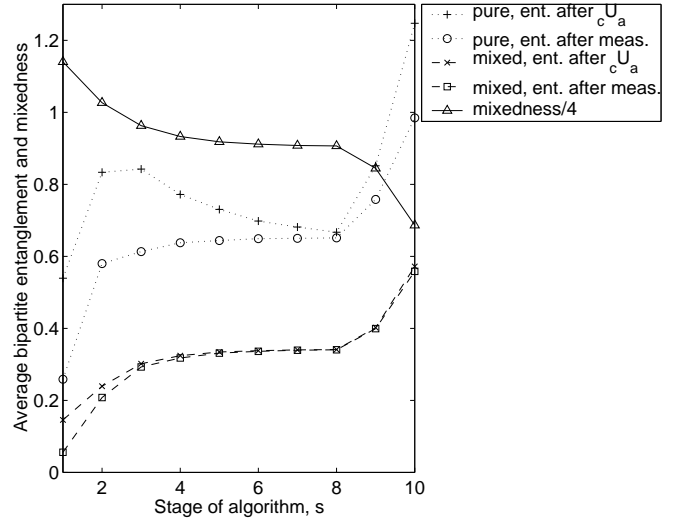


FIG. 6. As Fig. 5 but averaged over all algorithms for factorizing numbers which are products of two primes and have five binary digits (i.e. 21, 22, 25, 26) and over all possible numbers  $a$  coprime to each of these numbers.

These two sets of results have a very similar form, in particular the entanglement in the mixed state algorithms closely mirrors the mixedness of the quantum computer (the von Neumann entropy of the state of the whole computer) at each stage. Also note that the amount of entanglement increases towards then end of the algorithm where the most significant (i.e. the highest) bits of the number  $c$  are decided and the least significant bits of the period  $r$  are found.

We can see immediately that in all algorithms, both pure and mixed, according to our entanglement measure, entanglement exists although it is up to three times lower in Fig. 5 and 6 for the mixed state algorithm. The mixed state algorithms are, however, at least around half as efficient as the pure state algorithms for the values of  $N$  considered (which can be seen by calculating  $\frac{(p-1)(q-1)}{pq}$  for each  $N = pq$ ).

## B. Noise

Next we examine the effect of noise on particular algorithms, namely for  $N = 15$ ,  $a = 2$  (Figs. 7 and 8) which has period  $r = 4$  and  $N = 21$ ,  $a = 2$  (Figs. 9 and 10) which has period  $r = 6$ . Both measurement and Pauli noise were implemented as described in section V C. Additionally we considered the situation where the noise was not allowed to act on the control qubit.

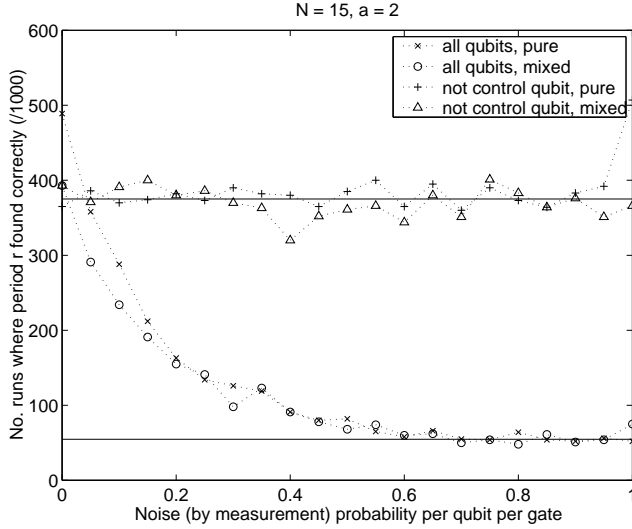


FIG. 7. The number of runs (out of 1000) of Shor's algorithm for  $N = 15$  and  $a = 2$  where the period,  $r$ , is found correctly (as calculated by a continued fractions algorithm) when noise, simulated by random measurements, is applied independently to each qubit. This number is plotted against the probability that a measurement is applied to each qubit after each gate in the algorithm. The plot contains both the pure and mixed state versions of Shor's algorithm and for noise applied to all of the qubits or all the qubits apart from the control qubit. Notice that when noise is not applied to the control qubit the algorithm becomes as efficient as the mixed state algorithm (upper solid line). This is because noise is not applied during the controlled modulo multiplication gates and the period is of the form  $r = 2^m$  where  $m$  is an integer. The lower solid line denotes the efficiency of a completely random algorithm.

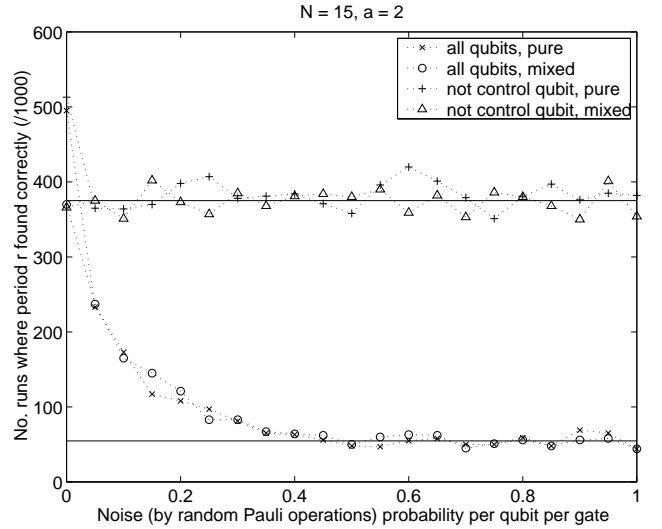


FIG. 8. As for Fig. 7 but where random Pauli operations are applied to each qubit after each gate with the given probability. Again notice that when noise is not applied to the control qubit the algorithm becomes as efficient as the mixed state algorithm.

For the  $N = 15$  case when noise is allowed to act on all qubits we see an exponential drop off in the efficiency of the algorithm with increasing noise level for both types of noise. However, when noise is not allowed to act on the control qubits the efficiency only falls to the efficiency level of the mixed state algorithm which, as has been noted, is efficient enough. The is due to the way the noise is implemented and the fact that the period is 4. For algorithms with period of the form  $r = 2^m$ , for some integer  $m$ , each of the controlled modulo multiplication gates can be applied on any state independently of the state of the system up to that point.

The reason is as follows: when the period is of the form  $2^m$  the first  $n - m$  controlled modulo multiplication gates are in fact the identity operation (note, however, that individual operations within the gate decomposition of the controlled modulo multiplications will not be the identity operation so noise would then greatly affect the efficiency of the algorithm) and the measurement result after each will be  $|0\rangle$ . The next gate is now the only relevant gate. If the measurement result after this gate is  $|1\rangle$  the period will be found correctly. In this case

$$c = \underbrace{????????}_{m-1 \text{ times}} \underbrace{1\,000\dots\dots000}_{n-m \text{ times}}. \quad (33)$$

where  $? = 0$  or  $1$ . Now, the fraction  $c/t$  will have denominator  $r$ , independent of the results of these  $m - 1$  remaining measurements.

Noise in the pure state algorithm applied to all but the control qubit, then, prepares these qubits in some random pure state (i.e. a mixed state). The first  $n - m$  stages of the algorithm do nothing but we will correctly find the

period if the next measurement result is  $|1\rangle$ , which will occur with the same probability as for the mixed state algorithm.

This is not the case for algorithms of other periods of course as the initial operations are not identity operations. An example is the  $N = 21$ ,  $a = 2$  algorithm for which the effects are noise are shown in Figs. 9 and 10

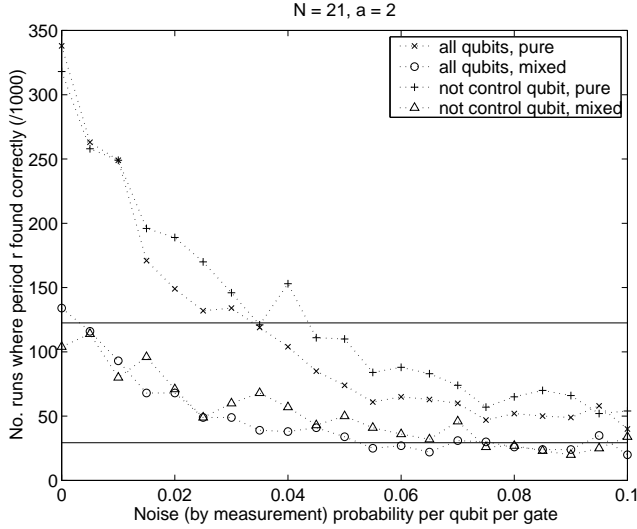


FIG. 9. As for Fig. 7 but for  $N = 21$  and  $a = 2$  where random measurement operations are applied to each qubit after each gate with a given probability. Here, when noise is not applied to the control qubit the algorithm is no longer as efficient as the mixed state algorithm, denoted by the upper solid line. The lower solid line shows the efficiency of a completely random algorithm.

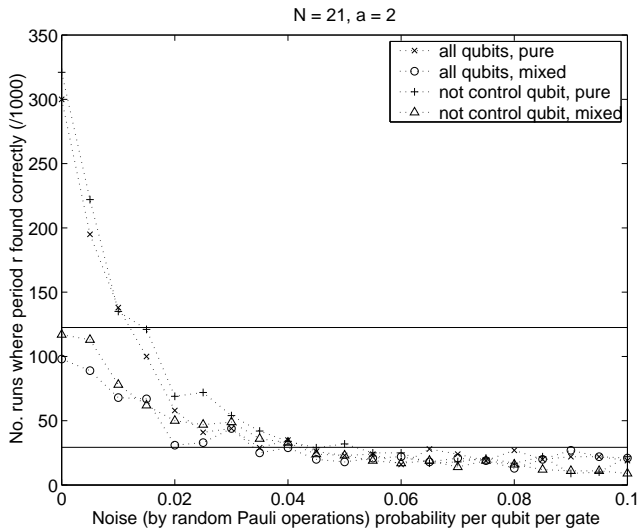


FIG. 10. As for Fig. 9 but where random Pauli operations are applied to each qubit after each gate with a given probability. Again notice that when noise is not applied to the control qubit the algorithm is no longer as efficient as the mixed state algorithm.

These results show us that for general algorithms we cannot increase the mixing of algorithms during its running by re-preparing another maximally mixed state in the lower register of qubits after each measurement without reducing the efficiency of the algorithm considerably - the previous measurements have prepared a state which must not be significantly altered before the next stage. If the period is of the form  $r = 2^m$  we can do this (although having a period of this form is presumably exponentially unlikely for increasing  $n = \log N$ ) but this will have no effect on the entanglement until the last  $m$  steps. For other algorithms this will reduce the entanglement but will also dramatically reduce the efficiency.

### C. Mixing of the control qubit

Let us now look at the effect of mixing the control qubit, as described in section VD. We will do this for both the 'pure' state algorithm (where all other qubits are initially pure) and the mixed state algorithm. Figs. 11 and 12 show the average bipartite entanglement throughout the entire algorithm versus the mixing parameter  $\epsilon$  for the pure and mixed state algorithms with  $N = 15$  and  $a = 2$  respectively. Also shown is the probability that each algorithm correctly finds the period,  $r$ .

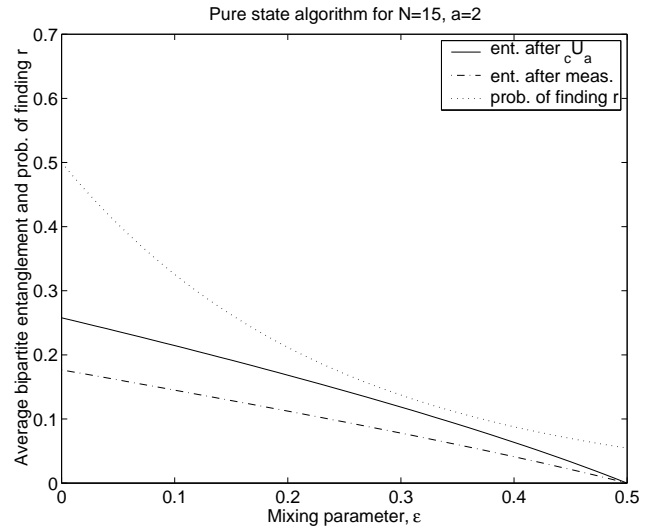


FIG. 11. Here we show, for the pure state algorithm of  $N = 15$  and  $a = 2$ , the entanglement averaged across all bipartite partitionings and all post  $-_c U_a$  and  $-$ measurement stages of the algorithm, vs. the mixing parameter,  $\epsilon$ , when the state of the control qubit is repeatedly prepared in the mixed state as in section VD. Also shown is the probability that the algorithm correctly finds the period  $r$ .

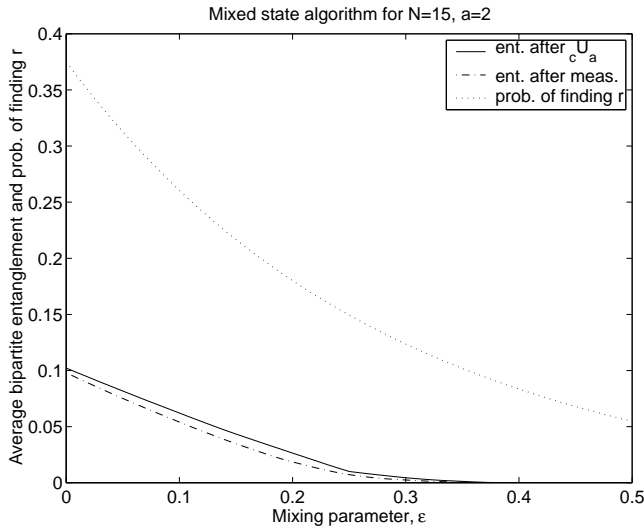


FIG. 12. As Fig. 11 but with the mixed state algorithm of  $N = 15$  and  $a = 2$ . Note that the average entanglement approaches zero before the algorithm is maximally mixed, where for the pure state algorithm it is zero only when the control qubit is maximally mixed ( $\epsilon = 0.5$ ).

Notice in particular how the entanglement in the mixed state algorithm approaches zero before the algorithm becomes entirely random. For the pure state algorithm it does not do so until  $\epsilon = 0.5$  is reached. The point at which the average entanglement is zero (to machine precision) in the mixed state algorithm is around  $\epsilon = 0.396$  for the  $N = 15$ ,  $a = 2$  case. This illustrates how the randomness in mixed states can completely mask the distillable entanglement even before the algorithm becomes entirely random. For the pure state case we have mixed two pure state algorithms (with orthogonal control qubit states), both of which do produce entanglement, and found that the entanglement does not disappear until we mix them maximally. For the mixed state algorithm we have also mixed two orthogonal algorithms which both contain entanglement but the distillable entanglement has been lost *before* we lose all information about which algorithm is running.

Compare these with similar results for the algorithms with  $N = 21$  and  $a = 2$  in Figs. 13 and 14.

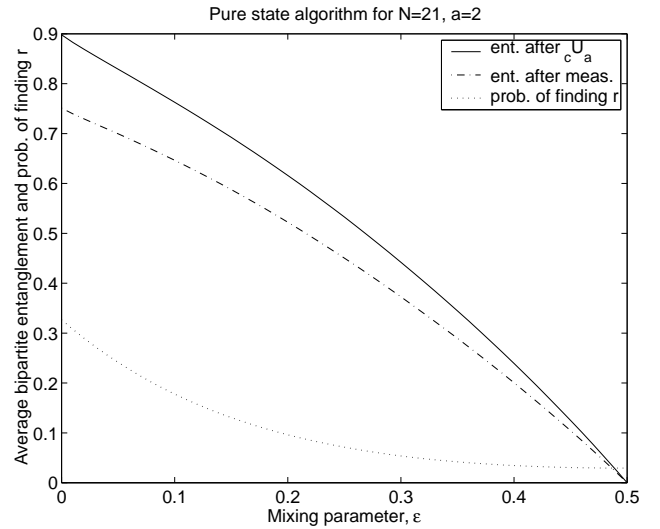


FIG. 13. For the pure state algorithm of  $N = 21$  and  $a = 2$ , the entanglement averaged across all bipartite partitionings and all post  $-_c U_a$  and -measurement stages of the algorithm, vs. the mixing parameter,  $\epsilon$ , when the state of the control qubit is repeatedly prepared in the mixed state as in section VD. Also shown is the probability that the algorithm correctly finds the period  $r$ .

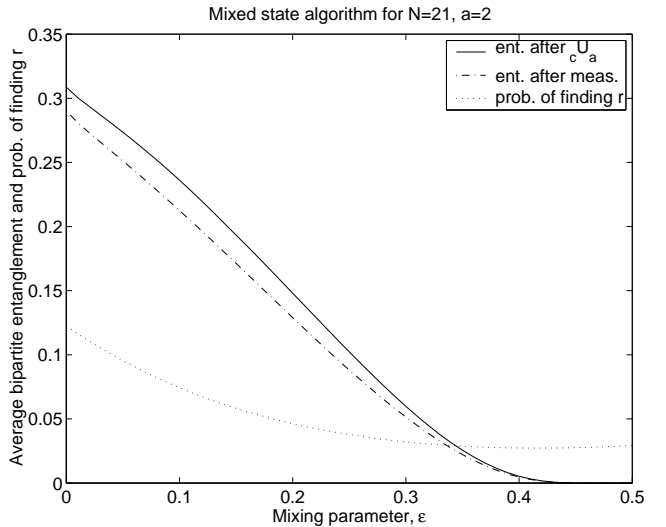


FIG. 14. As Fig. 13 but with the mixed state algorithm of  $N = 21$  and  $a = 2$ . Again note that the average entanglement approaches zero before the algorithm is maximally mixed. The point at which the entanglement is lost occurs for a higher value of  $\epsilon$  than for the then  $N = 15$  algorithm.

Again we see that the entanglement in the mixed state algorithm is zero before the control qubit is maximally mixed, although this point occurs at the higher value of around  $\epsilon = 0.470$ .

Finally we combine the results above to plot the probability of finding  $r$  against the average entanglement. This is shown in Figs. 15 and 16.

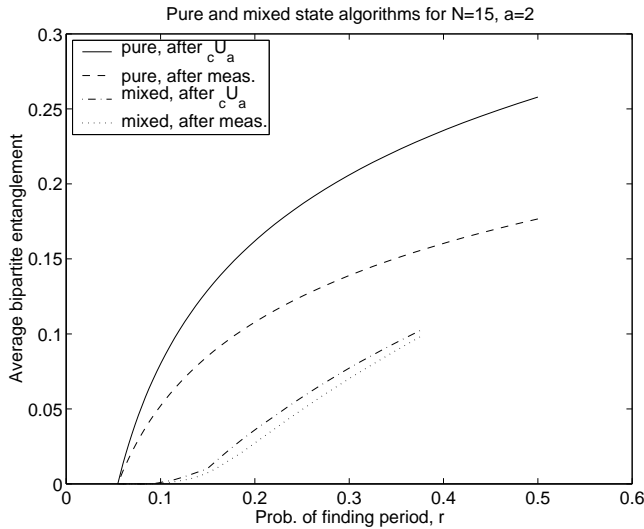


FIG. 15. Here we show the same set of results as Fig. 11 and 12 but we have plotted the probability of correctly finding the period  $r$  against the average bipartite entanglement.

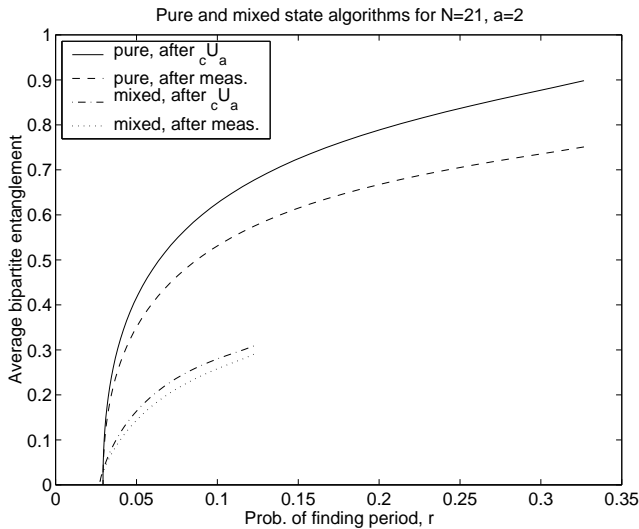


FIG. 16. Here we show the same set of results as Fig. 13 and 14 but we have plotted the probability of correctly finding the period  $r$  against the average bipartite entanglement.

For each particular algorithm, then, we see a definite trend of an increase in entanglement giving an increase in the probability of correctly finding the period, although initially increasing the entanglement from zero does not produce such a large increase in this probability. We also see that the entanglement required for a given probability is lower for the mixed state algorithm. The maximal probability of correctly finding the period is of course lower for the mixed state algorithm but in the limits  $p, q \rightarrow \infty$  this is negligibly so.

## VII. CONCLUSIONS

It has been shown that it is possible to efficiently factorize with Shor's algorithm using only one initially pure qubit and a supply of initially maximally mixed qubits. We have also seen that for algorithms with small numbers of qubits the mixing of the algorithm remains high throughout. It is then a natural question to see whether any entanglement is involved in the execution of the quantum algorithm. We find that the high degree of mixing, however, does not preclude the existence of entanglement and indeed in these example algorithms entanglement does appear to exist, even when the state of the computer starts and remains in a highly mixed state.

Conversely, if we try to reduce this entanglement by introducing further mixing into the control qubit we do reduce the entanglement in the computer but at the expense of a reduction in efficiency of the computation. The mixing of the control qubit also sheds light on the nature of entanglement itself, that is, we do not need to lose all information about the nature of an entangled state before we are completely unable to extract entanglement from it, as we have seen when mixing two orthogonal entangled mixed state algorithms.

We have also seen that Shor's algorithm operated on mixed states is nevertheless susceptible to noise of different kinds and the algorithm does not in general appear to have any increased robustness to noise (except where the noise model on particular algorithms is too simplified to be accurate) even though this algorithm can be run using highly mixed states.

What remains an open question is as to how the above effects behave for algorithms of increasing numbers of qubits. Presumably the entanglement does remain for algorithms of large numbers of qubits and the algorithm remains highly susceptible to noise but because of the exponential nature of simulating the algorithms verifying this is an extremely difficult task.

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